

# **Adaptive Modeling of Thermal Non-Equilibrium in Two-Phase Flow Simulation Systems**

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## **1 Introduction**

Multiphase flow simulation systems used nowadays in nuclear engineering consider a fully developed thermal non-equilibrium. Computer codes as RELAP5 consider two phases. Both phases might have temperatures that differ from the respective saturation temperature.

Irreversible thermodynamics is the physics of thermal non-equilibrium. Though irreversible thermodynamics and multiphase simulation investigate similar arrangements, no attempt has made so far to apply principles of irreversible thermodynamics to multiphase flow simulation.

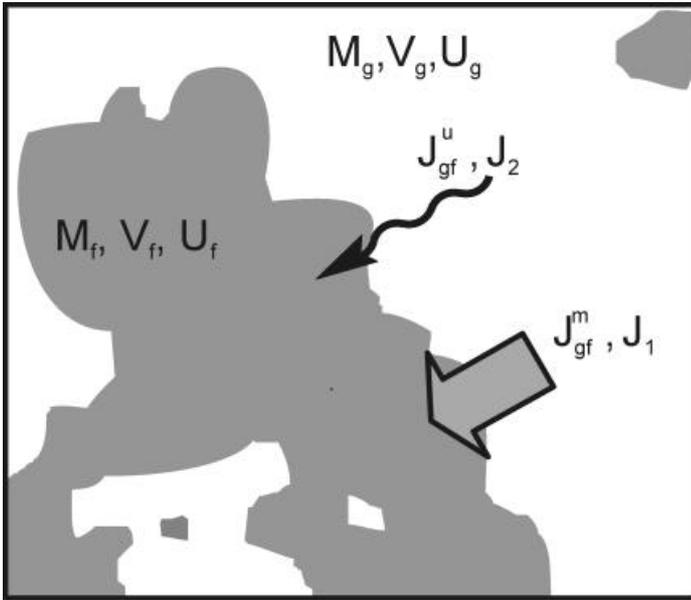
In this presentation the conception of “adaptive modeling” is introduced. Adaptive modeling considers the existing modeling of constitutive relations and applies irreversible thermodynamics absolutely direct. In general, application of irreversible thermodynamics reduces the number of constitutive relations by imposing constraints on them. The consideration will be focused on the application of Onsager’s theorem of reciprocity.

After presenting some elementary concepts of irreversible thermodynamics, adaptive modeling is applied to interface mass and heat transfer, and afterwards to wall heat transfer and the associated mass transfer.

## 2 Irreversible Thermodynamics in a Two-Phase System

### 2.1 Concepts of Irreversible Thermodynamics

Irreversible thermodynamics (Callen 1960; Becker 1985; Meixner 1959) can be considered as a theory about entropy production. In the following, this conception will be applied to an adiabatic one-component system composed of a liquid and a gaseous phase, which is shown in Fig. 1:



**Fig. 1: Mass and heat fluxes in an adiabatic two-phase system**

The thermal state is fully described by its extensive parameters: Liquid mass  $M_f$ , liquid internal energy  $U_f$ , liquid volume  $V_f$ , gaseous mass  $M_g$ , gaseous internal  $U_g$ , and gaseous volume  $V_g$ , with the entropy  $S$  being a function of those quantities:

$$S = S(M_f, U_f, V_f, M_g, U_g, V_g) \quad (1)$$

The entropy production rate is given by the total derivative of the entropy with respect to time:

$$\frac{dS}{dt} = \left( \frac{\partial S_L}{\partial M_L} - \frac{\partial S_G}{\partial M_G} \right) \frac{dM_L}{dt} + \left( \frac{\partial S_L}{\partial U_L} - \frac{\partial S_G}{\partial U_G} \right) \frac{dU_L}{dt} + \left( \frac{\partial S_L}{\partial V_L} - \frac{\partial S_G}{\partial V_G} \right) \frac{dV_L}{dt} \quad (2)$$

In the expression on the right-hand side, the closure of the system is already considered, as any increase of an extensive parameter of the liquid phase corresponds to the identical reduction of the respective parameter of the gaseous phase.

The derivatives of entropy with respect to the extensive system parameters are fundamental thermodynamical parameters.

$$F_1^* = \frac{\partial S_f}{\partial M_f} - \frac{\partial S_g}{\partial M_g} = - \left( \frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) \quad (3)$$

$$F_2^* = \frac{\partial S_f}{\partial U_f} - \frac{\partial S_g}{\partial U_g} = \frac{1}{T_f} - \frac{1}{T_g} \quad (4)$$

$$F_3^* = \frac{\partial S_f}{\partial V_f} - \frac{\partial S_g}{\partial V_g} = \frac{p_f}{T_f} - \frac{p_g}{T_g} \quad (5)$$

The rates of change of the extensive parameters are named as fluxes by definition. The fluxes occurring in Eq. (2) are

$$J_1^* = \frac{dM_f}{dt} = - \frac{dM_g}{dt} \quad (6)$$

$$J_2^* = \frac{dU_f}{dt} = - \frac{dU_g}{dt} \quad (7)$$

$$J_3^* = \frac{dV_f}{dt} = - \frac{dV_g}{dt} \quad (8)$$

Forces and fluxes are causally connected. At least close to thermal equilibrium, it is reasonable to establish a linear dependence of the fluxes on the forces. Higher order dependencies can be formulated (Callen, 60), but no practical applications are given.

For the isolated two-phase system under consideration, the fluxes have the following representation:

$$J_i^* = \sum_{k=1,2,3} L_{ik}^* F_k^* \quad i=1,2,3 \quad (9)$$

At this point, Onsager's reciprocity theorem becomes effective. The theorem expresses that when the flux, corresponding to the irreversible process  $i$ , is influenced by the affinity  $F_k$  of the irreversible process  $k$  through  $L_{ik}$ , then the flux  $k$  is influenced by the affinity  $F_k$  through the same coefficient (Prigogine, 55).  $L^*$  forms a symmetric matrix:

$$L_{ik}^* = L_{ki}^* \quad i,k = 1,2,3 \quad (10)$$

By insertion of Eq. (3) through Eq. (5), the following basic form for the fluxes presenting the interface heat and mass transfer is received:

$$J_1^* = -L_{11}^* \left( \frac{\mu_f}{T_f} - \frac{\mu_{fg}}{T_{fg}} \right) + L_{12}^* \left( \frac{1}{T_f} - \frac{1}{T_g} \right) + L_{13}^* \left( \frac{p_f}{T_f} - \frac{p_g}{T_g} \right) \quad (11)$$

$$J_2^* = -L_{12}^* \left( \frac{\mu_f}{T_f} - \frac{\mu_{fg}}{T_{fg}} \right) + L_{22}^* \left( \frac{1}{T_f} - \frac{1}{T_g} \right) + L_{23}^* \left( \frac{p_f}{T_f} - \frac{p_g}{T_g} \right) \quad (12)$$

$$J_3^* = -L_{13}^* \left( \frac{\mu_f}{T_f} - \frac{\mu_{fg}}{T_{fg}} \right) + L_{23}^* \left( \frac{1}{T_f} - \frac{1}{T_g} \right) + L_{33}^* \left( \frac{p_f}{T_f} - \frac{p_g}{T_g} \right) \quad (13)$$

The linear coefficients are designated as kinetic coefficients. As indicated above, they form a symmetric matrix.

## 2.2 The "Hydrostatic Assumption"

In the previous section, fluxes have been formulated with consideration of a complete thermal non-equilibrium. Contemporary simulation techniques describe multiphase systems by thermal and chemical non-equilibrium, whereas mechanic equilibrium is assumed. With exception of stratified flow, the pressures are homogeneous within the phases. Ransom (1989) to describe this type of thermal states firstly used the term "hydrostatic assumption".

$$p_f = p_g = p \quad (14)$$

For the mass flux, dependence on the phase dependent pressures can be eliminated:

$$J_1^M = J_1^* = -L_{11}^* \left( \frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) + (L_{12}^* + pL_{13}^*) \left( \frac{1}{T_f} - \frac{1}{T_g} \right) \quad (15)$$

For the use in simulation systems as RELAP5, it is appropriate to combine the fluxes of Eqs. (12) and (13) :

$$J_2^{U+pV} = J_2^* + pJ_3^* = -(L_{12}^* + pL_{13}^*) \left( \frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) + (L_{22}^* + 2pL_{23}^* + p^2L_{33}^*) \left( \frac{1}{T_f} - \frac{1}{T_g} \right) \quad (16)$$

With substitutions

$$L_{11} = L_{11}^* \quad (17)$$

$$L_{12} = L_{12}^* + pL_{13}^* \quad (18)$$

$$L_{22} = L_{22}^* + 2pL_{23}^* + p^2L_{33}^* \quad (19)$$

we receive a set of two fluxes, which constitute the set of source terms in the balance equations as used in RELAP5.

$$J_1 = -L_{11} \left( \frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) + L_{12} \left( \frac{1}{T_f} - \frac{1}{T_g} \right) = L_{11}F_1 + L_{12}F_2 \quad (20)$$

$$J_2 = -L_{12} \left( \frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) + L_{22} \left( \frac{1}{T_f} - \frac{1}{T_g} \right) = L_{12}F_1 + L_{22}F_2 \quad (21)$$

$J_1$  is the source term in the mass balance equation,  $J_2$  the source term in the energy balance. It is remarkable; that the symmetry that was imposed by Onsager's reciprocity relations to the original coefficient matrix (Eqs. (11) through (13)) is conserved. With

respect to the second law of thermodynamics, the symmetry of the matrix allows simple mathematical formulations for the positive-definiteness of a quadratic form, which can be constructed to describe the entropy generation rate.

### 2.3 Single-Component Systems

In nuclear engineering, analysis was historically focused on single-component systems consisting by water and steam. Models, which consider a non-condensable component in the gaseous phase, are still in a developmental stage, the effects of a soluble component in the liquid phase on the thermal behavior have not considered yet. Because of their importance, the general form of the fluxes as derived in Eq. (20) and Eq. (21) will be evaluated subsequently for one-component systems.

Evaluation profits by the existence of a saturation line, which exclusively exists in a two-phase system with a single component. By the saturation line for a given pressure, a saturation temperature  $T_{\text{sat}}$  is determined. Thermal properties of a thermal non-equilibrium state can be mathematically expanded with respect to pressure and respective saturation temperature.

With the abbreviations

$$dT_{\text{sf}} = T_{\text{sat}} - T_{\text{f}} \quad (22)$$

and

$$dT_{\text{sg}} = T_{\text{sat}} - T_{\text{g}} \quad (23)$$

an approximation of force  $F_2$ , Eq. (4),

$$F_2 = \frac{1}{T_{\text{f}}} - \frac{1}{T_{\text{g}}} = \frac{T_{\text{sat}} + dT_{\text{sf}}}{(T_{\text{sat}} - dT_{\text{sf}})(T_{\text{sat}} + dT_{\text{sf}})} - \frac{T_{\text{sat}} + dT_{\text{sg}}}{(T_{\text{sat}} - dT_{\text{sg}})(T_{\text{sat}} + dT_{\text{sg}})} \quad (24)$$

is obtained by neglecting second order terms:

$$F_2 = \frac{1}{T_f} - \frac{1}{T_g} = \frac{1}{T_{sat}^2} (dT_{sf} - dT_{sg}) \quad (25)$$

A transformation for the force  $F_1$ , Eq. (3), can be performed by using the thermal relation

$$\frac{\partial}{\partial T} \left( \frac{\mu}{T} \right)_p = -\frac{h}{T} \quad (26)$$

This generates the following approximation:

$$\frac{\mu_f(p, T_f)}{T_f} = \frac{\mu_f(p, T_{sat})}{T_{sat}} + \frac{h_{f,sat}}{T_{sat}^2} dT_{sf} \quad (27)$$

A similar relation holds for the gaseous phase. As thermal potentials of liquid and gas are equal for saturation conditions, the respective force has the following form:

$$F_1 = - \left( \frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) = \frac{-1}{T_{sat}^2} (h_{f,sat} dT_{sf} - h_{g,sat} dT_{sg}) \quad (28)$$

We apply Eq. (25) and Eq. (28) and recalculate the fluxes of Eqs. (20) and (21), and we receive a direct dependence on the deviations of liquid and gas temperatures from the saturation temperature:

$$J_1^M = \frac{1}{T_{sat}^2} \left[ (-L_{11} h_{f,sat} + L_{12}) dT_{sf} - (-L_{11} h_{g,sat} + L_{12}) dT_{sg} \right] \quad (29)$$

$$J_2^{U+pV} = \frac{1}{T_{sat}^2} \left[ (-L_{12} h_{f,sat} + L_{22}) dT_{sf} - (-L_{12} h_{g,sat} + L_{22}) dT_{sg} \right] \quad (30)$$

The application of these fluxes in a system simulation requires the determination of three kinetic coefficients  $L_{11}$ ,  $L_{12}$ , and  $L_{22}$ . They form the set of constitutive relations, which describe interface mass and heat transfer when considering principles of irreversible thermodynamics.

## 2.4 Adaptive Modeling of Interface Mass and Heat Transfer

Mass flux  $J_1^M$  corresponds to the negative “interface evaporation rate”  $\Gamma_{ig}$  in the traditional modeling, as defined in the RELAP5-3D manual (R3D-Team 2001, Eq. 3.1-28), which reads:

$$\Gamma_{ig} = -\frac{H_{if}}{h_g^* - h_f^*} dT_{sf} - \frac{H_{ig}}{h_g^* - h_f^*} dT_{sg} \quad (31)$$

The associated interface heat transfer rate is given by (R3D-Team 2001, e.g. Eqs. (3.1-78) or (3.1-79))

$$Q_{ig} = -\frac{h_g^* H_{if}}{h_g^* - h_f^*} dT_{sf} - \frac{h_f^* H_{ig}}{h_g^* - h_f^*} dT_{sg} \quad (32)$$

Contrary to the definition in this paper used when defining the fluxes of irreversible thermodynamics, the rates as defined in RELAP5 are positive if they are directed towards the steam phase.

In the traditional modeling, four constitutive coefficients exist:  $H_{if}$ ,  $H_{ig}$ ,  $h_f^*$ ,  $h_g^*$ . The enthalpies depend on the sign of the evaporation rate.

Adaptive modeling investigates the correspondence of the fluxes defined by Eq. (29) and Eq. (30), and of the rates defined by Eq. (31) and Eq. (32). Obviously, both representations depend linearly on the deviations of the phase temperatures from the saturation temperatures. The representations correspond, if the coefficients are identical:

$$\frac{-L_{11} h_{f,sat} + L_{12}}{T_{sat}^2} = \frac{H_{if}}{h_g^* - h_f^*} \cdot V \quad (33)$$

$$\frac{+L_{11} h_{g,sat} - L_{12}}{T_{sat}^2} = \frac{H_{ig}}{h_g^* - h_f^*} \cdot V \quad (34)$$

$$\frac{-L_{12}h_{f,\text{sat}} + L_{22}}{T_{\text{sat}}^2} = \frac{h_g^* H_{if}}{h_g^* - h_f^*} \cdot V \quad (35)$$

$$\frac{+L_{12}h_{g,\text{sat}} - L_{22}}{T_{\text{sat}}^2} = \frac{h_f^* H_{ig}}{h_g^* - h_f^*} \cdot V \quad (36)$$

With given right hand sides, Eqs. (33) and (34) form a set of linear equations which allow determining  $L_{11}$  and  $L_{12}$ . By the set of linear equations formed by Eqs. (35) and (36),  $L_{12}$  and  $L_{22}$  can be calculated. Thus, two expressions for  $L_{12}$  are received.

$$L_{12}(\text{mass}) = -\frac{V \cdot T_{\text{sat}}^2 (h_{f,\text{sat}} H_{ig} + h_{g,\text{sat}} H_{if})}{(h_g^* - h_f^*)(h_{g,\text{sat}} - h_{f,\text{sat}})} \quad (37)$$

$$L_{12}(\text{energy}) = -\frac{V \cdot T_{\text{sat}}^2 (h_f^* H_{ig} + h_g^* H_{if})}{(h_g^* - h_f^*)(h_{g,\text{sat}} - h_{f,\text{sat}})} \quad (38)$$

Obviously, both expressions are identical, if and only if

$$h_f^* = h_{f,\text{sat}} \quad (39)$$

$$h_g^* = h_{g,\text{sat}} \quad (40)$$

Adaptive modeling of interface mass and heat transfer affects the formulation of enthalpies  $h_f^*$  and  $h_g^*$ . If they are set to their respective saturation temperature, Onsager's reciprocity relation is fulfilled, and the modeling is in accordance to the principles of irreversible thermodynamics.

### 3 Adaptive Modeling of Boiling

#### 3.1 Irreversible Thermodynamics and Wall Heat Transfer

Application of irreversible thermodynamics to the modeling of boiling for use in thermal-hydraulic simulation systems will be subsequently described by considering the most primitive thermal system where boiling can occur. It consists by a two-phase fluid, which is in thermal contact with an adjacent wall. A schematic view is given by Fig. 2:

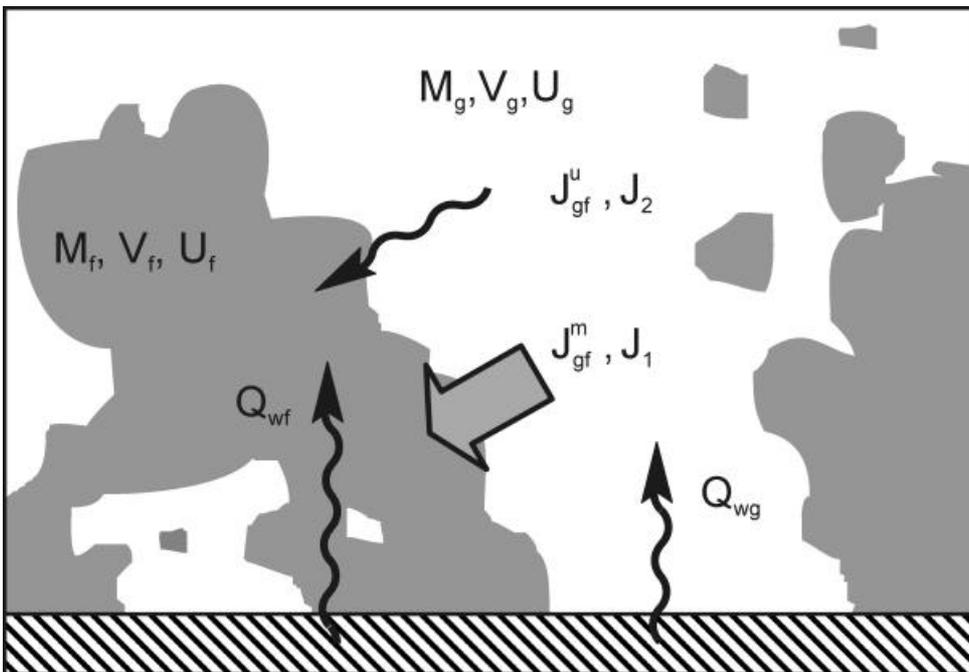


Fig. 2: Fluxes in a two-phase system with an adjacent wall

The thermal state of this system is fully described by its extensive parameters. Six parameters are necessary to describe the two phases of the fluid. For use in simulation systems, the thermal state of the wall is defined by its internal energy. Compressibility of the wall is neglected.

The prediction of the thermal history by means of irreversible thermodynamics proceeds for the generation rate of the entropy of the total system.

$$\begin{aligned} \frac{dS}{dt} = & \left( \frac{\partial S_f}{\partial M_f} - \frac{\partial S_g}{\partial M_g} \right) \frac{\partial M_f}{\partial t} + \left( \frac{\partial S_f}{\partial V_f} - \frac{\partial S_g}{\partial V_g} \right) \frac{\partial V_f}{\partial t} \\ & + \frac{\partial S_f}{\partial U_f} \frac{\partial U_f}{\partial t} + \frac{\partial S_g}{\partial U_g} \frac{\partial U_g}{\partial t} + \frac{\partial S_w}{\partial U_w} \frac{\partial U_w}{\partial t} \end{aligned} \quad (41)$$

The fluxes can be derived similar to the procedure as presented in Section 2.2. We receive:

$$J_1 = -L_{11} \left( \frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) + L_{12} \left( \frac{1}{T_f} - \frac{1}{T_g} \right) + L_{13} \left( \frac{1}{T_f} - \frac{1}{T_w} \right) + L_{14} \left( \frac{1}{T_g} - \frac{1}{T_w} \right) \quad (42)$$

$$J_2 = -L_{12} \left( \frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) + L_{22} \left( \frac{1}{T_f} - \frac{1}{T_g} \right) + L_{23} \left( \frac{1}{T_f} - \frac{1}{T_w} \right) + L_{24} \left( \frac{1}{T_g} - \frac{1}{T_w} \right) \quad (43)$$

$$J_3 = -L_{13} \left( \frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) + L_{23} \left( \frac{1}{T_f} - \frac{1}{T_g} \right) + L_{33} \left( \frac{1}{T_f} - \frac{1}{T_w} \right) + L_{34} \left( \frac{1}{T_g} - \frac{1}{T_w} \right) \quad (44)$$

$$J_4 = -L_{14} \left( \frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) + L_{24} \left( \frac{1}{T_f} - \frac{1}{T_g} \right) + L_{34} \left( \frac{1}{T_f} - \frac{1}{T_w} \right) + L_{44} \left( \frac{1}{T_g} - \frac{1}{T_w} \right) \quad (45)$$

As schematically presented in Fig. 2,  $J_1$  represents the mass flux from the gaseous into the liquid phase.  $J_2$  represents the associated interface heat transfer.  $J_3$  presents the heat transfer from the wall into the liquid phase. And  $J_4$  represents the heat transfer from the wall into the gaseous phase. For one-component systems, transformations of Eqs. (28) and (24) become effective and the set of fluxes which will be used as basis for the adaptive modeling reads:

$$J_1 = \frac{1}{T_{\text{sat}}^2} \left[ \left( -L_{11} h_{f,\text{sat}} + L_{12} \right) dT_{\text{sf}} - \left( -L_{11} h_{g,\text{sat}} + L_{12} \right) dT_{\text{sg}} + L_{13} (T_w - T_f) + L_{14} (T_w - T_g) \right] \quad (46)$$

$$J_2 = \frac{1}{T_{\text{sat}}^2} \left[ \left( -L_{12} h_{f,\text{sat}} + L_{22} \right) dT_{\text{sf}} - \left( -L_{12} h_{g,\text{sat}} + L_{22} \right) dT_{\text{sg}} + L_{23} (T_w - T_f) + L_{24} (T_w - T_g) \right] \quad (47)$$

$$J_3^{wf} = \frac{1}{T_{sat}} \left[ \left( -L_{13} h_{f,sat} + L_{23} \right) dT_{sf} - \left( -L_{13} h_{g,sat} + L_{23} \right) dT_{sg} + L_{33} (T_w - T_f) + L_{34} (T_w - T_g) \right] \quad (48)$$

$$J_4^{wg} = \frac{1}{T_{sat}} \left[ \left( -L_{14} h_{f,sat} + L_{24} \right) dT_{sf} - \left( -L_{14} h_{g,sat} + L_{24} \right) dT_{sg} + L_{34} (T_w - T_f) + L_{44} (T_w - T_g) \right] \quad (49)$$

In total 10 kinetic coefficients show up and have to be determined empirically. With reference to adaptive modeling, Onsager's reciprocity relations generate five constraints by the off-diagonal elements, which reduce the number of independent constitutive relations.

### 3.2 Nucleate Boiling

The heat transfer rate of nucleate boiling is described by Chen's correlation. If only a one component gas is considered, it reads:

$$q_{nucleate} = h_{mic} (T_w - T_{sat}) + h_{mac} (T_w - T_f) \quad (50)$$

In the standard modeling, heat transfer takes place exclusively between wall and liquid phase. As no heat is transferred into the gaseous phase, in the adaptive modeling,  $J_4$  is zero; so  $L_{14}$ ,  $L_{24}$ ,  $L_{34}$ , and  $L_{44}$  must be zero likewise.

Eq. (48) describes the heat transfer between wall and liquid based on irreversible thermodynamics. The flux depends on temperature differences  $T_{sat}-T_f$ ,  $T_{sat}-T_g$ , and  $T_w-T_f$  - but not on  $T_w-T_{sat}$ . Therefore Eq. (50) is reformulated:

$$q_{nucleate} = -h_{mic} (T_{sat} - T_f) + 0 \cdot (T_{sat} - T_g) + (h_{mic} + h_{mac}) (T_w - T_f) \quad (51)$$

Adaptive modeling of nucleate boiling starts with comparing the structure of the heat transfer rate as given by Chen and the heat flux between wall and liquid derived with consideration of irreversible thermodynamics. Adaptive modeling assumes that Eqs. (48) and (51) correspond. Three temperature differences are included; and the respective coefficients have to be equal.

$$\frac{1}{T_{\text{sat}}} (-L_{13} h_{f,\text{sat}} + L_{23}) = -h_{\text{mic}} A_{\text{wall}} \quad (52)$$

$$L_{13} h_{g,\text{sat}} - L_{23} = 0 \quad (53)$$

$$L_{33} = (h_{\text{mic}} + h_{\text{mac}}) A_{\text{wall}} \quad (54)$$

The equations allow determining the kinetic coefficients  $L_{13}$ ,  $L_{23}$ , and  $L_{33}$ . Eq. (54) forms no constraint, as  $L_{33}$  shows up only once. Though being determined by analyzing the structure of the heat transfer correlation, because of the assumed validity of Onsager's relations,  $L_{13}$  occurs in the mass flux and represents the amount of vaporization due to the wall heat transfer.  $\Gamma_w$ , which is this vaporization term in RELAP5-3D, can be therefore expressed as a function of the kinetic coefficient  $L_{13}$ , and subsequently as a function of  $h_{\text{mic}}$ . It is

$$\Gamma_w = -\frac{1}{V} L_{13} (T_w - T_f) = \frac{A_{\text{wall}}}{(h_{g,\text{sat}} - h_{f,\text{sat}}) V} h_{\text{mic}} (T_w - T_f) \quad (55)$$

Consequently, within adaptive modeling the structure of the heat transfer correlation given by Eq. (50) determines the vaporization.

It is worth to compare this result with the standard modeling. In modern code versions, there is a tendency to model  $\Gamma_w$  quite independent from  $h_{\text{mic}}$ . In the modeling of RELAP5/MOD2, a close connection between heat and mass transfer exists. The heat, which transfers from the wall into the fluid, is divided. A defined fraction generates vapor. Therefore, this term is a function of the temperature difference between wall and saturation temperature, according to the formulation of the heat transfer rate. Application of irreversible thermodynamics teaches that though a common coefficient  $h_{\text{mic}}$  is used for the calculation of heat and mass transfer,  $h_{\text{mic}}$  is multiplied by  $T_w - T_{\text{sat}}$  when calculating the heat transfer rate. But when calculating the vaporization term caused by this heat transfer,  $h_{\text{mic}}$  has to be multiplied by  $T_w - T_f$ . Obviously, this approach promotes the evaporation during subcooled nucleate boiling, as the temperature difference in the mass source term is increased.

The enthalpy transport during boiling can be derived by Eq. (53), as  $L_{23}$  appears in  $J_2$ , which represents the interface heat transfer. It is

$$h_{\text{transport}} = h_{\text{g,sat}} \quad (56)$$

This is in correspondence with the standard modeling. The close connection to the kinetic coefficient  $L_{23}$  demonstrates that this enthalpy is a constitutive term. Therefore, its determination is always nontrivial – as will be demonstrated in the next section.

### 3.3 Film Boiling

In RELAP5-3D heat transfer of film boiling is described by the modified Bromley correlation:

$$q_{\text{film}} = h_{\text{film}} (T_w - T_{\text{sat}}) + h_v (T_w - T_g) \quad (57)$$

In the standard modeling, heat transfer takes place exclusively between wall and liquid phase. However, Eq. (57) depends on  $T_w - T_g$ . As indicated by name, film boiling is associated with a vapor film between wall and fluid core. Therefore it is highly reasonable to assume that the heat from the wall is exclusively transmitted into the vapor phase. Again, Eq. (57) has to be slightly converted:

$$q_{\text{film}} = 0 \cdot (T_{\text{sat}} - T_f) - h_{\text{film}} (T_{\text{sat}} - T_g) + (h_{\text{film}} + h_v) (T_w - T_g) \quad (58)$$

Comparing coefficients in this equation with respective coefficients of Eq. (49) generates two equations:

$$-\frac{1}{T_{\text{sat}}} (-L_{14} h_{\text{f,sat}} + L_{24}) = -h_{\text{film}} A_{\text{wall}} \quad (59)$$

$$L_{14} h_{\text{f,sat}} - L_{24} = 0 \quad (60)$$

Again, application of Onsager's reciprocity relations allows to determine  $\Gamma_w$ .

$$\Gamma_w = -\frac{1}{V} L_{14} (T_w - T_g) = \frac{A_{\text{wall}}}{(h_{g,\text{sat}} - h_{f,\text{sat}}) V} h_{\text{film}} (T_w - T_g) \quad (61)$$

and generates a formulation of the transport enthalpy. It is:

$$h_{\text{transport}} = h_{g,\text{sat}} \quad (62)$$

As already stated, the determination of this enthalpy is nontrivial. For simple conditions, it is a saturation enthalpy. If heat from the wall flows exclusively into the liquid phase, it is the saturation enthalpy of liquid, if heat is transmitted into the vapor phase, it is the saturation temperature of steam.

## 4 Summary

Within a simulation system for multiphase flow, the modeling of processes, which occur with thermal non-equilibrium, is of central importance. Those processes comprise mass and heat transfer between the phases and wall induced boiling and condensation. Irreversible thermodynamics can provide an understanding of the pertinent phenomena.

Adaptive modeling is the straightforward application of irreversible thermodynamics to existing simulation systems. Without any additional assumptions, constraints emerge from the assumed validity of Onsager's reciprocity theorem which reduce the number of constitutive relations and generate a modeling approach which is strongly based on physical principles.

## Availability Notice

In Germany and other European countries, patents are granted. A patent in the United States is pending.

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